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Diffusion in a crowded environment

Andrzej Sikorski[1]*, Piotr Polanowski[2]

[1]Faculty of Chemistry, University of Warsaw, Pasteura 1, 02-093 Warsaw, Poland
[2]Department of Molecular Physics, Łódź University of Technology, 90-924 Łódź, Poland
*sikorski@chem.uw.edu.pl

We present results of extensive and systematic simulation studies of two-dimensional fluid motion in a complex crowded environment. In contrast to other studies we focused on cooperative phenomena that occurred if the motion of particles takes place in a dense crowded system, which can be considered as a crude model of a cellular membrane. Our main goal was to answer a fundamental question: how do the fluid molecules move in a disordered environment with a complex structure. The influence of crowding is especially interesting in two-dimensional cases, e.g. in membranes where the presence of macromolecules, proteins and cytoskeleton often changed the mobility, and anomalous diffusion appeared [1]. The dynamic lattice liquid (DLL) model, which can work at the highest fluid density, was employed for this purpose [2]. This model became a basis for a parallel algorithm which took into account coincidences of elementary molecular motion attempts resulting in local cooperative structural transformations. Within the frame of the DLL model we considered systems that contained mobile and immobile objects of various kinds [3-4]. The dynamic properties of the system were studied. The subdiffusive motion of fluid molecules was found in the crowded system and described. The simulation and the analysis emphasize the influence of the movement correlation between moving particles and obstacles.

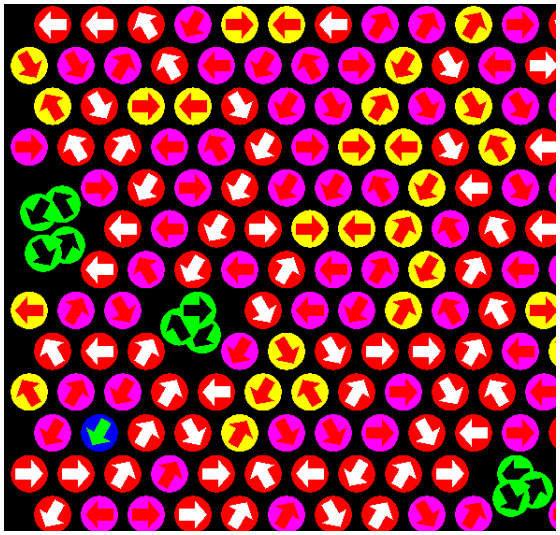

Figure 1: A scheme of the DLL model: collisions (yellow), vacant creations (red), open paths (pink), and closed motion paths (green).

References

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